ELECTRONIC SUPPLEMENTARY MATERIAL (ESI) FOR NEW JOURNAL OF CHEMISTRY

Supporting Information

Conformational studies on substituted ε-caprolactams by X-ray crystallography and NMR spectroscopy

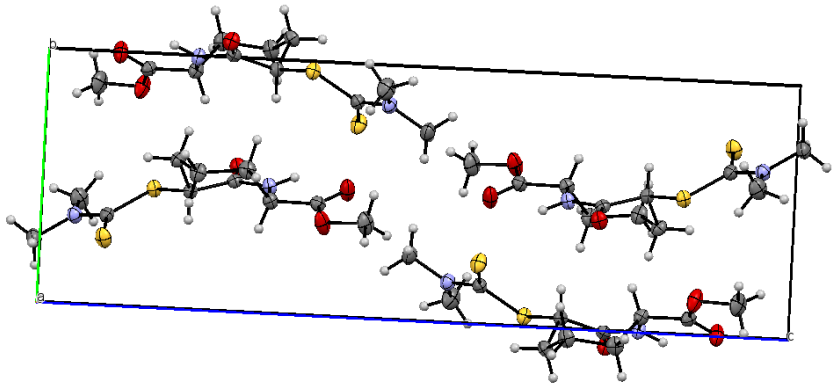
Tobias Gruber,[a,*] Amber L. Thompson,[a] Barbara Odell,[a] Petra Bombicz,[b] Christopher J. Schofield[a,*]

[a] University of Oxford, Department of Chemistry, Chemistry Research Laboratory, 12 Mansfield Road, Oxford OX1 3TA, United Kingdom. E-mail: christopher.schofield@chem.ox.ac.uk; Fax: +44 1865 285002; Tel: +44 1865 275625 or tobias.gruber@chemie.tu-freiberg.de; Tel: +49 3731 392390

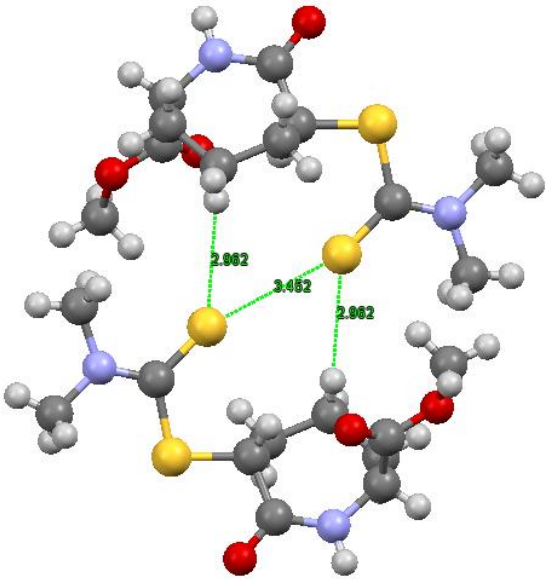
[b] Institute of Organic Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Magyar Tudósok körútja 2., H-1117 Budapest, Hungary

Table S1
Distances (Å) and angles (°) of hydrogen bond type interactions in the here discussed X-ray structures

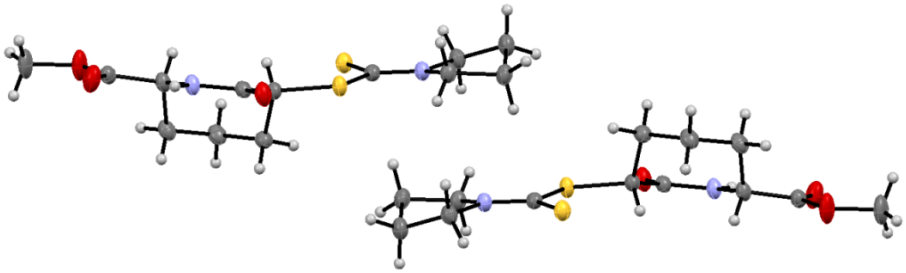
Atoms involved	Distance (Å)				Angle (°)
	Symmetry	d(D-H)	d(H...A)	d(D...A)	<(DHA)
1					
N(1)-H(11)...O(1)	-*x*+2, -*y*, -*z*+2	0.85	2.25	3.056(3)	160
C(6)-H(61)...O(1)	*x*-1, *y*, *z*	0.98	2.52	3.498(3)	174
C(8)-H(81)...O(2)	*x*-1, *y*, *z*	0.95	2.52	3.258(3)	134
2					
N(1A)-H(1A)...O(2C)	*x*, *y*, *z*	0.85	2.14	2.970(4)	164
O(3A)-H(3A)...O(1A)	*x*, *y*, *z*	0.82	1.75	2.555(4)	169
N(1B)-H(1B)...O(2A)	*x*, *y*, *z*	0.85	2.18	2.996(4)	162
O(3B)-H(3B)...O(1C)	*x*, *y*, *z*	0.84	1.72	2.543(4)	170
N(1C)-H(1C)...O(2B)	*x*, *y*, *z*	0.85	2.25	3.074(4)	162
O(3C)-H(3C)...O(1A)	*x*, *y*, *z*	0.85	1.72	2.553(4)	170
3					
C(6)-H(61)...O(2)	-*x*+1, -*y*, -*z*+1	0.95	2.57	3.341(2)	139
5 *cis*					
C(2)-H(21)...O(1)	-*x*+2, *y*+1/2, -*z*+3/2	0.97	2.52	3.392(2)	150
C(4)-H(42)...O(3)	-*x*+1, *y*-1/2, -*z*+3/2	0.96	2.50	3.331(2)	144
C(5)-H(52)...O(1)	*x*-1, *y*, *z*	0.98	2.44	3.279(2)	143
C(6)-H(61)...O(1)	-*x*+2, *y*+1/2, -*z*+3/2	0.95	2.51	3.363(2)	150
5 *trans*					
N(1)-H(11)...O(1)	-*x*+1, -*y*+1, -*z*+2	0.87	2.00	2.868(4)	176
C(6)-H(61)...O(2)	*x*, *y*, *z*	0.97	2.42	3.157(4)	132
C(10)-H(101)...O(2)	-*x*+2, -*y*, -*z*+1	0.95	2.40	3.235(4)	147
6 *cis*					
C(2)-H(21)...O(1)	-*x*+3/2, *y*+1/2, -*z*+1/2	0.94	2.56	3.4627(2)	162
C(4)-H(42)...O(3)	-*x*+1/2, *y*-1/2, -*z*+1/2	0.94	2.51	3.3072(2)	143
C(5)-H(52)...O(1)	*x*-1, *y*, *z*	0.95	2.55	3.4293(2)	154
7					
N(1)-H(11)...O(1)	-*x*+2, -*y*+2, -*z*+1	0.88	1.98	2.862(2)	179
C(2)-H(21)...O(1)	-*x*+2, -*y*+1, -*z*+1	0.96	2.47	3.410(2)	168
C(6)-H(61)...O(2)	-*x*+1, -*y*+2, -*z*+2	0.97	2.50	3.277(2)	138



a)



b)



c)

Fig. S1 Packing behaviour of dithiocarbamates *cis*-**5** (a), *trans*-**5** (b) and *cis*-**6** (c).